A revised model for microbially induced calcite precipitation - improvements and insights

International Research Training Group nupus

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Motivation

With increasing intensity of subsurface use, ensuring separation between different layers with competitive uses becomes more and more important. The risk of polluting upper layers, e.g. used for drinking water production, by applications such as CO_2 storage in the subsurface or fracking could be reduced with sealing technologies like microbially induced calcite precipitation (MICP). Other applications of MICP are discussed in Phillips et al. (2013).

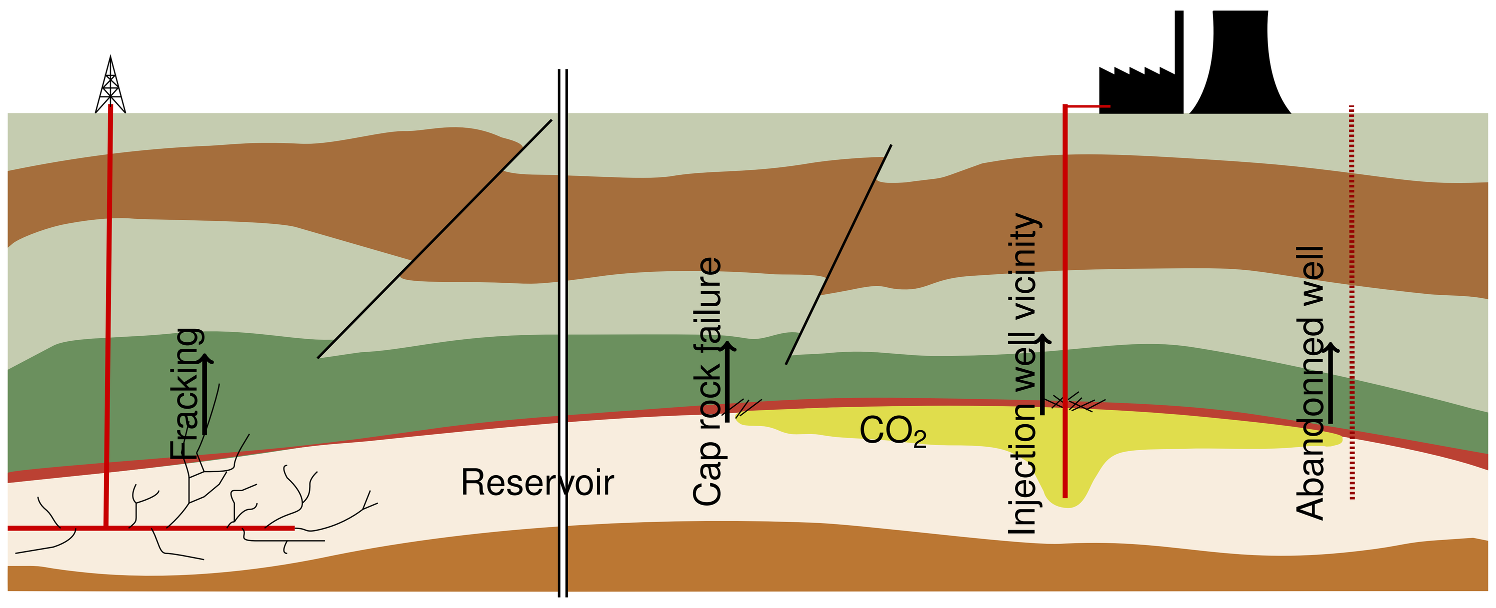

Figure 1 : *Potential application sites of MICP as a sealing technology in the subsurface.*

Model concept

The REV-scale MICP model includes reactive two-phase multi-component transport including two solid phases.

$$\text{solid phases: } \frac{\partial}{\partial t}(\phi_\lambda \rho_\lambda) = q^\lambda_{\text{reactions}}$$

$$\text{solutes: } \sum_\alpha \left[\frac{\partial}{\partial t}(\phi \rho_\alpha x^\kappa_\alpha S_\alpha) + \nabla\cdot(\rho_\alpha x^\kappa_\alpha \mathbf{v}_\alpha) - \nabla\cdot\left(\rho_\alpha \mathbf{D}_{\text{pm},\alpha} \nabla x^\kappa_\alpha\right)\right] = q^\kappa_{\text{reactions}}$$

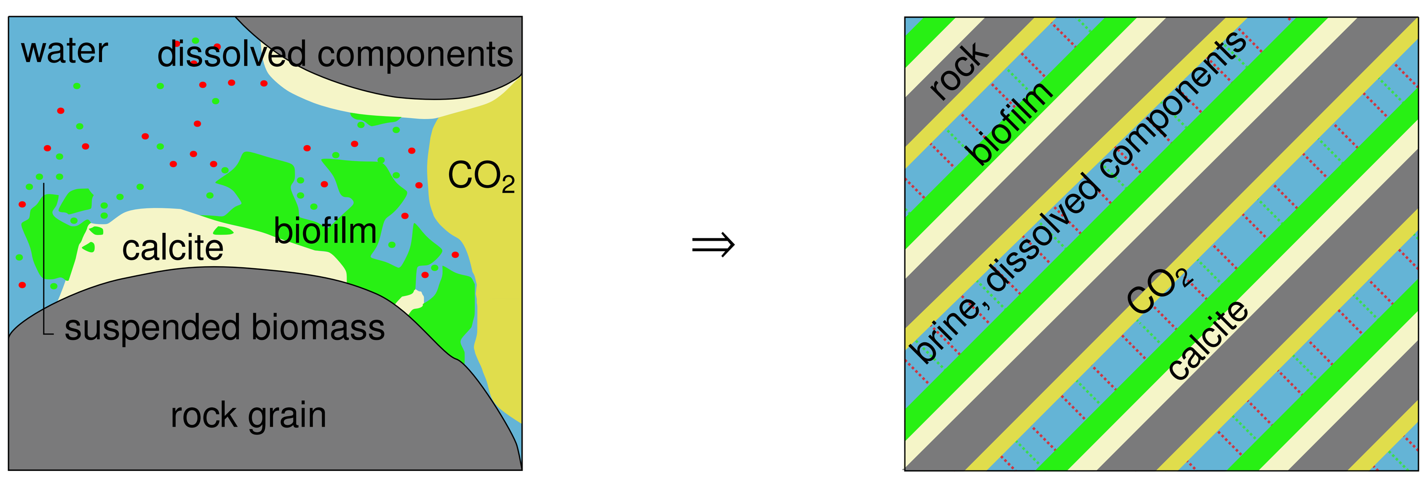

Figure 2 : *Model relevant phases and distribution of components in the phases at pore scale and REV-scale, modified from Ebigbo et al. (2012).*

Relevant processes

Several bio- and geo-chemical processes, in combination with solute transport, are important for MICP:

- two-phase multi-component flow
- processes determining the distribution of biomass:
  - growth: $r_{\text{growth}} = \mu\, \rho_{\text{biofilm}}\, \phi_{\text{biofilm}} \frac{C_w^{O_2}}{C_w^{O_2}+K_{O_2}} \frac{C_w^{\text{substrate}}}{C_w^{\text{substrate}}+K_{\text{substrate}}}$,
  - decay: $r_{\text{decay}} = k_{\text{decay}}\, \rho_{\text{biofilm}}\, \phi_{\text{biofilm}}$,
  - attachment: $r_{\text{attachment}} = (c_{a,1}\, \phi_{\text{biofilm}} + c_{a,2})\, S_w\, \phi\, C_w^{\text{bacteria}}$,
  - detachment: $r_{\text{detachment}} = c_{d,1}\, (S_w\, \phi\, |\nabla p_w|)^{0.58} + c_{d,2}\, \mu$,
- (bio-) chemical reactions:
  - microbially catalyzed ureolysis: $CO(NH_2)_2 + 2\,H_2O \xrightarrow{\text{urease}} 2\,NH_3 + H_2CO_3$,
  - influence of NH_3 on the pH: $NH_3 + H^+ \leftrightarrow NH_4^+ \Rightarrow$ increase in pH,
  - precipitation (and dissolution) of calcite: $Ca^{2+} + CO_3^{2-} \leftrightarrow CaCO_3 \downarrow$,

    $r_{\text{precipitation}} = k_{\text{precipitation}}\, A_{sw}\, (\Omega - 1)^{n_{\text{precipitation}}}$,

    which is depended on the calcite saturation state $\Omega = \frac{[Ca^{2+}][CO_3^{2-}]}{K_{sp}}$ and the water-solid surface area A_{sw}.
- clogging: $\phi = \phi_0 - \phi_{\text{calcite}} - \phi_{\text{biofilm}} \Rightarrow K = K_0 \left(\frac{\phi - \phi_{\text{crit}}}{\phi_0 - \phi_{\text{crit}}}\right)^3$

DuMux Simulations are performed using the open-source simulator DuMux.

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Link to this poster.

Model improvement

Improved ureolysis rate equation

In recent kinetic studies on the ureolysis by *Sporosarcina pasteurii*,

$$CO(NH_2)_2 + 2\,H_2O \xrightarrow{\text{urease}} 2\,NH_3 + H_2CO_3$$

kinetic parameters were determined by Lauchnor et al. (2015). The improved knowledge is used to update the numerical model replacing the previously used ureolysis rate equation (Ebigbo et al., 2012):

$$r_{\text{urea, old}} = \frac{k_{\text{urease}}}{1+\frac{m^{H^+}}{K_{\text{eu},1}}+\frac{K_{\text{eu},1}}{m^{H^+}}}\, k_{\text{ub}}\, (\rho_{\text{biofilm}}\, \phi_{\text{biofilm}})^{n_{\text{ub}}}\, \frac{m^{\text{urea}}}{m^{\text{urea}}+K_{\text{urea}}}\, \frac{K_{NH_4^+}}{m^{NH_4^+}+K_{NH_4^+}}$$

with the new rate equation according to experiments with whole cells of *S. pasteurii* (Lauchnor et al., 2015), which is independent of NH_4^+ and H^+ concentrations:

$$r_{\text{urea, new}} = k_{\text{urease, new}}\, k_{\text{ub, new}}\, \rho_{\text{biofilm}}\, \phi_{\text{biofilm}}\, \frac{m^{\text{urea}}}{m^{\text{urea}}+K_{\text{urea, new}}}.$$

Model recalibration

The improved implementation of ureolysis causes a need to refit the model, since the updated kinetic parameters are significantly different from the previously used ones. Instead of trial-and-error methods, this recalibration is conducted using inverse modeling. Fitted parameters are the biofilm density ρ_{biofilm}, the attachment coefficient of bacteria to biofilm $c_{a,1}$, the attachment coefficient of bacteria to arbitrary solid surfaces $c_{a,2}$, and the urease content of the biofilm $k_{\text{ub, new}}$.

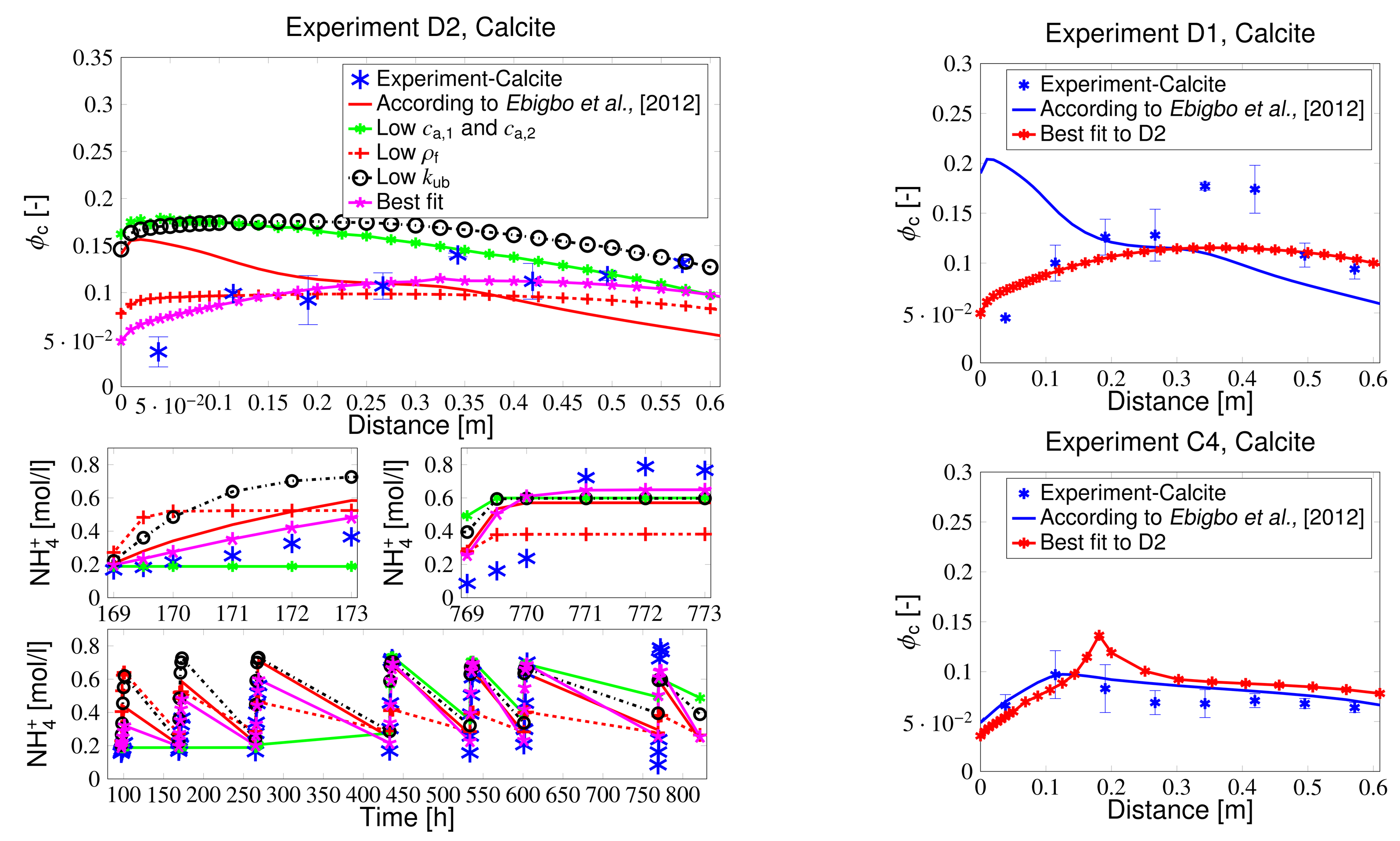

Figure 3 : *Comparison of the model predictions for different sets of parameters obtained by inverse modeling for the experiment D2 (Hommel et al., 2015) used to calibrate the parameters (left, top: calcite, bottom: NH_4^+). On the right, the predictions using the parameter set "best fit" are compared with predictions by the previous model (Ebigbo et al., 2012) and the results of two different column experiments, D1 (Hommel et al., 2015) (top) and C4 (Ebigbo et al., 2012) (bottom).*

Summary

- Implemented more realistic, but also simplified ureolysis kinetics;
- Improved fit to new column experiments (D1, D2);
- Predictions for old column experiments (C4), as published in Ebigbo et al. (2012); confirm the range of the *Ebigbo* model;
- Most sensitive parameter is the urease content of the biofilm $k_{\text{ub, new}}$;
- Revised model published in Hommel et al. (2015).

Literature

Anozie Ebigbo, Adrienne J Phillips, Robin Gerlach, Rainer Helmig, Alfred B Cunningham, Holger Class, and Lee H Spangler. Darcy-scale modeling of microbially induced carbonate mineral precipitation in sand columns. *Water Resources Research*, 48(7):W07519, July 2012. doi: 10.1029/2011WR011714.

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